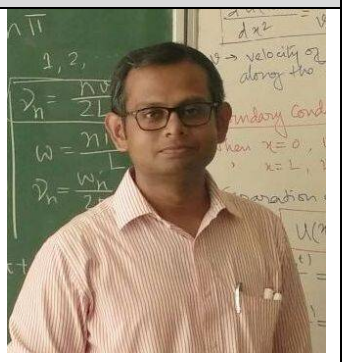
CENTRAL UNIVERSITY OF JAMMU

First Name	Tapta	Middle Name	KANCHAN	Last Name	ROY	
Title & Designation		Dr. Assistant Professor				
Address		Department of Chemistry and Chemical Sciences Central University of Jammu Rahya-Suchani (Bagla), District-Samba Jammu-181143, J&K, India				
Phone Number						
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Email		tapta.che@cujammu.ac.in				
Web-Page		http://www.cujammu.ac.in//5105/Default.aspx?option=article&type=single&id=20373&mnuid=21425&prvt				

Educational Qualifications: PhD

Degree	Institution	Year
B. Sc.	Presidency College, University of Calcutta	2002
M.Sc.	Banaras Hindu University	2004
CSIR-NET-JRF		2006
PhD	School of Chemistry, University of Hyderabad	2011

Career Profile:

1. August 2016 - present:
Assistant Professor, Department of Chemistry & Chemical Sciences, Central University of Jammu, Jammu

2. January 2015- May 2016
Assistant Professor, Department of Chemistry, Central University of Rajasthan, Rajasthan

3. August 2012 - December 2014
Post Doctoral Research Fellow, Fritz Heber Research Center for Molecular Dynamics, The Hebrew University of Jerusalem, Israel

4. August 2011 - June 2012
Post Doctoral Research Fellow, Computational Material Chemistry Division, Ruhr University, Bochum, Germany

5. March 2011 - May 2011
Research Associates, School of Chemistry, University of Hyderabad

Administrative Assignments:

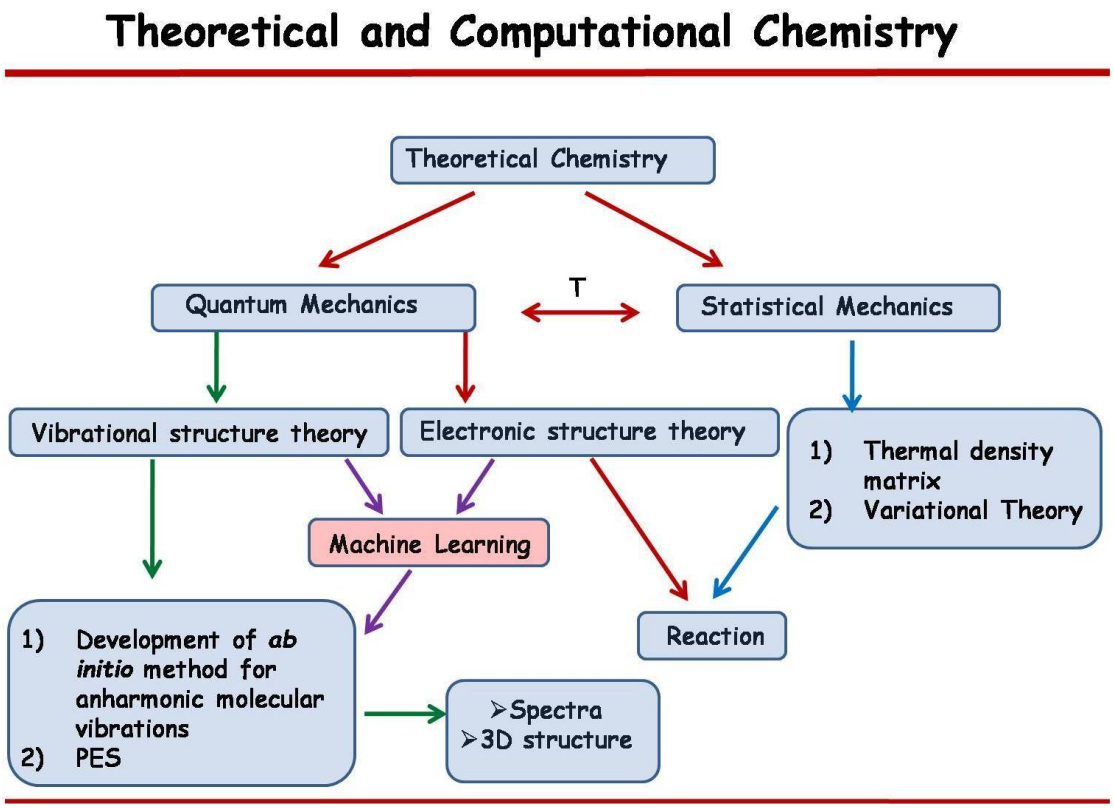
1) Department Coordinator, CUJ (2017-2020)
2) Research Advisory Committee, Department of Environmental Science and Department of Molecular Biology, CUJ (2021-)
3) BoS member, Department of Chemistry and Chemical Sciences, CUJ (2018-2020)
4) BoS member, Department of Physics and Astronomical Sciences, CUJ (2020-2023)
5) DRC member of the Department of Chemistry and Chemical Sciences, CUJ (2018-2020, 2023-present)

6) Member, Departmental Purchase Committee
7) Member, Departmental Technical committee
8) Member, Technical Verification committee
9) Member, Departmental affairs committee
10) Departmental representative, DIQA, CUJ

Areas of Interest / Specialization:

Physical Chemistry :: Theoretical and Computational Chemistry

- Development of new formalism for quantum anharmonic vibrational spectroscopy and their applications
- Developments of Artificial intelligent based Machine Learning algorithms for ro-vibrational spectroscopy
- Developments of potential energy surfaces
- Many-body theory
- Quantum statistical mechanics for temperature depended properties
- Development of computational chemistry software
- Molecular understanding of $H^+/H/H^-$ migrations

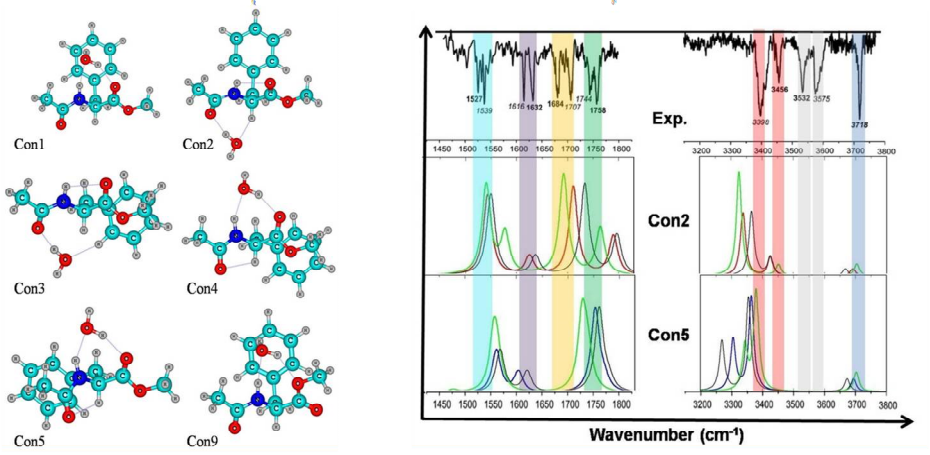


Anharmonic Molecular Vibrations: VSCF-PT2 approximation

$$\Psi(Q_1,\ldots,Q_N) = \prod_{i=1}^{N} \psi_i^{(n)}(Q_i) \quad . \qquad (1)$$

$$\left[-\frac{1}{2}\frac{\partial^2}{\partial Q_i^2} + \overline{V_i^{(n)}}(Q_i)\right]\psi_i^{(n)} = \epsilon_i^{(n)}\psi_i^{(n)}(Q_i) \, . \qquad (2)$$

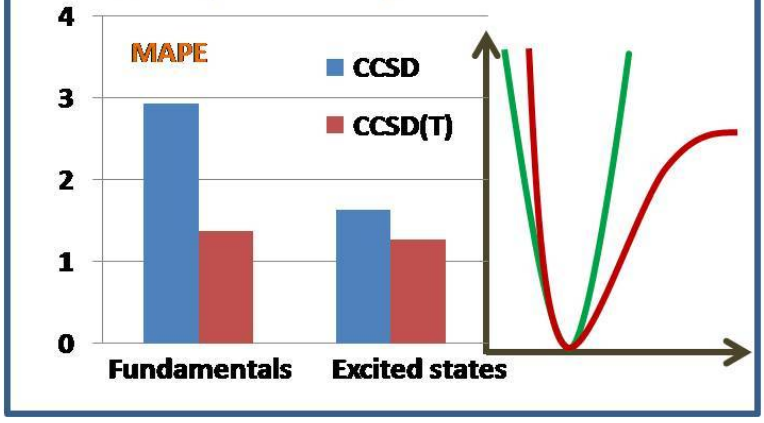
$$\overline{V_i^{(n)}}(Q_i) = \left\langle \prod_{j\neq i}^{N} \psi_j^{(n)}(Q_j) \middle| V(Q_1,\ldots,Q_N) \middle| \prod_{j\neq i}^{N} \psi_j^{(n)}(Q_j) \right\rangle . \qquad (3)$$



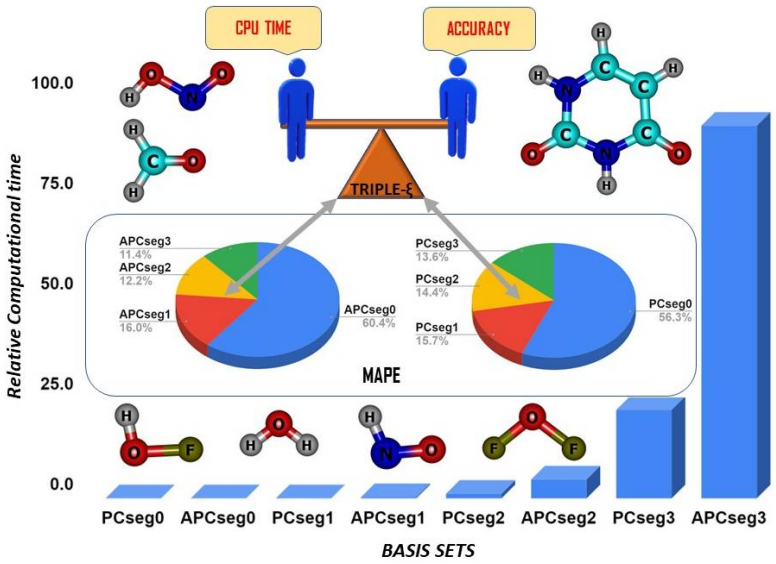
Accuracy of Potential Energy Surface

VSCF-PT2 : $\overline{V_i^{(n)}}(Q_i) = \left\langle \prod_{j\neq i}^{N} \psi_j^{(n)}(Q_j) \middle| V(Q_1,\ldots,Q_N) \middle| \prod_{j\neq i}^{N} \psi_j^{(n)}(Q_j) \right\rangle$

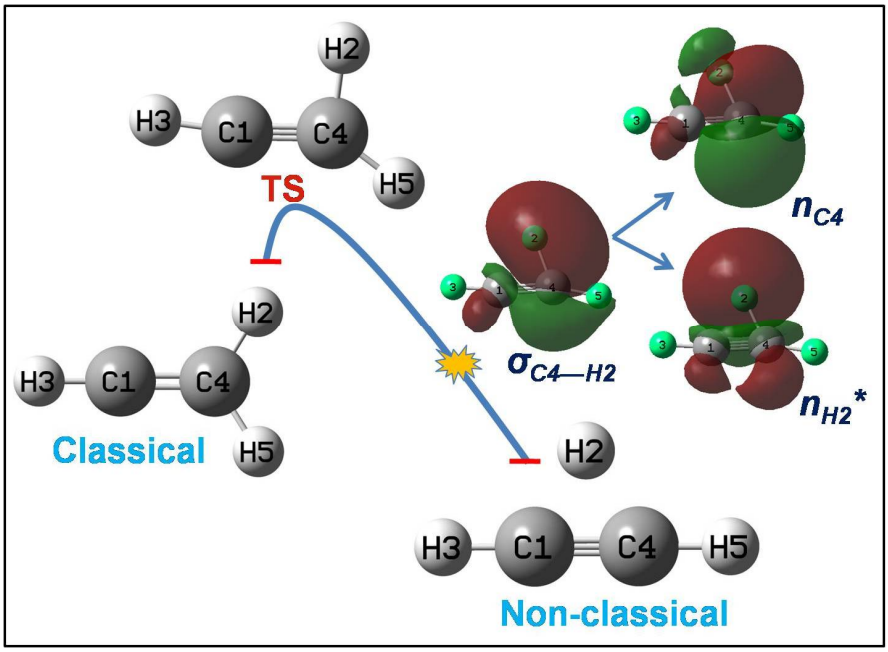
CC : $|\psi> = e^T|\Phi_0>$



Benchmark Study on hardware efficient computations of quantum vibrational algorithms



Proton Shuttle Motion



Subjects Taught:

- **PhD Level:**

1) Computer Programming and Numerical Methods
2) Advanced Quantum Mechanics and Computational Chemistry

- **UG & PG level**

1) General Chemistry-I
2) General Chemistry-II
3) General Chemistry Lab-I
4) General Chemistry Lab-II
5) Physical Chemistry-I
6) Physical Chemistry-II
7) Physical Chemistry Lab-I
8) Physical Chemistry Lab-I
9) Inorganic Chemistry Lab-II
10) Dissertation (VI semester)
11) Quantum Mechanics, Surface & Colloid Chemistry
12) Spectroscopy & Computational Chemistry
13) Group Theory & Spectroscopy
14) Quantum Chemistry & Chemical Dynamics.
15) Thermodynamics, Kinetics and Spectroscopy lab

Research Guidance:

One completed, two ongoing

Publications Profile:

Total No. of Publications: 43 (International Journals, peered reviewed)
Total Citations: > 1120 (Google scholar)
h-index: 20
i10 index = 25

a. **Research Papers**

43. Accuracy of Different Electronic Basis Set Families for Anharmonic Molecular Vibrations: A Comprehensive Benchmark Study
D. Sharma and **T. K. Roy***
J. Phys. Chem. A, (2023), 127, 7132–7147, ISSN: 1520-5215, https://doi.org/ 10.1021/acs.jpca.3c02874

42. The importance of electron correlations on vibrational anharmonicitiesand potential energy surfaces

A. Fayaz, S. Banik and **T. K. Roy***
Comput. Theor. Chem., (2023), 122, 114059, ISSN: 2210-271X, https://doi.org/10.1016/j.comptc.2023.114059

41. Sulfonated Polybenzimidazole as a PEM in a Microbial Fuel Cell: An Efficient Strategy for Green Energy Generation and Wastewater Cleaning

S. Subhadarshini, J. S. Sravan, O. Sarkar, S. V. Mohan, **T. K. Roy** and T. Jana
ACS Appl. Energy Mater., (2023) 6, 1422–1438, ISSN: 2574-0962, https://doi.org/10.1021/acsaem.2c03238

40. Effects of non-local exchange functionals in the density functional theories forthe description of molecular vibrations

    A. Fayaz, **T. K. Roy,***and S.Banik,*
    J. Chem Sc., 134, 67 (2022), ISSN: 0973-7103, https://doi.org/10.1007/s12039-022-02061-1

39. Performance of Vibrational Self-Consistent Field Theory for Accurate Potential Energy Surfaces: Fundamentals, Excited States, and Intensities.

    T. K. Roy*
    J. Phys. Chem. A, 2022, 126, 608–622, ISSN: 1520-5215, https://doi.org/10.1021/acs.jpca.1c09989

38. Halloysite nanotubes functionalized sulfonic acid: synthesis, spectroscopic characterization, computational studies and application for the synthesis of 1,4-dihydropyridines

    P. Gupta,*N. Prakash, Y. Ramawat, P. Rajput, A. Fayaz, **T. K. Roy***
    Lett. Org.Chem., 19, 19, (2022) ISSN: 1875-6255, https://doi.org/10.2174/1570178618666210302160130

37. Porphyrin bearing phenothiazine pincers as hosts for fullerene binding via concave–convex complementarily: synthesis and complexation study

    K. Jain, N.Duvva, **T. K. Roy**,* L.Giribabu* and R. Chitta*
    New J. Chem., 45, 19691–19703 (2021), ISSN: 1144-0546, https://doi.org/10.1039/D1NJ03727G

36. Rhodium(III)-Catalyzed Annulation of 2-Arylimidazo[1,2-a]pyridines with Maleimides: Synthesis of 1H-Benzo[e]pyrido[1′,2′:1,2]imidazo[4,5-g]isoindole-1,3(2H)-Diones and their Photophysical Studies

    V. N. Shinde, **T. K. Roy**, S. Jaspal, D. S. Nipate, N. Meena, K. Rangan, D. Kumar, A. Kumar
    Adv. Synth. Catal., (2020), 362, 5751-5764,ISSN 1615-4169, https://doi.org/10.1002/adsc.202000960

35. Comprehensive Benchmark Results to the Accuracy of Basis Sets for the Anharmonic Molecular Vibrations

    H. Mitra and **T. K. Roy***
    J. Phys. Chem. A, (2020), 124, 44, 9203–9221, ISSN: 1520-5215, https://doi.org/10.1021/acs.jpca.0c06634

34. Dual Basis Approach for Ab Initio Anharmonic Calculations of Vibrational Spectroscopy: Application to Micro-Solvated Biomolecules

    T. K. Roy* and R. B. Gerber.
    J. Chem. Theory Comput. (2020), 16, 11, 7005–7016, ISSN: 1549-9618, https://doi.org/10.1021/acs.jctc.0c00725

33. Comprehensive Analysis of Band Gap and Nanotwinning in $Cd_{1-x}Mg_xS$ QDs

T. Kalsi, H. Mitra, **T. K. Roy**, S. K. Godara and P. Kumar
Cryst. Growth Des. (2020), 20, 10, 6699–6706, ISSN**:** 1528-7483, https://doi.org/10.1021/acs.cgd.0c00851

32. On the Proton Shuttle Motion in Protonated Acetylene: AnElectronic Structure Perspective

S. Banik, A. K. Sansi, S. Nandan. and **T. K. Roy***
ChemistrySelect, (2020)*5*, 9288 –9295, **ISSN**:2365-6549, https://doi.org/10.1002/slct.202002524

31. Dinuclear gold(I)-N-heterocyclic carbene complexes: Synthesis, characterization, and catalytic application for hydrohydrazidation of terminal alkynes

S. Yadav, S. Ray, A Singh, S. M. Mobin, **T. K. Roy***, C. Dash.
Appl. Organomet. Chem., (2020) 34, e5942, ISSN**:** 1099-0739, https://doi.org/10.1002/aoc.5942

30. Conjugated Small Organic Molecules: Synthesis and Characterization of 4-Arylpyrazole-decorated Dibenzothiophenes

S. Panda, R. S. Jat, A. Fayaz, J. Saha, R. Thirumoorthi, **T. K. Roy** and M. Bhanuchandra
New J. Chem., (2020) 44,8944-8951, ISSN: 1144-0546, https://doi.org/10.1039/D0NJ01887B

29. Designed Synthesis, Characterization and Evaluation of Anticancer Activity of Water-Soluble Half-sandwich Ruthenium (II)Arene Halido Complexes

T. A. Khan, K. Bhar, R. Thirumoorthi, **T. K. Roy*** and A. K. Sharma*
New J. Chem., 44, 239-257 (2020), ISSN: 1144-0546, https://doi.org/10.1039/C9NJ03663F

28. Novel axially ligated complexes of Zn(II)porphyrin: spectroscopic, computational, and antibiological characterization

S. Kundan, G. D.Bajju, D. Gupta, **T. K. Roy**
Russian J. Inorg. Chem.,*64*, 1379–1395 (2019),ISSN: 1531-8613, https://doi.org/10.1134/S003602361911010X

27. Intrinsic Structure of Pentapeptide Leu-enkephalin: Geometry Optimization and Validation by Comparison of VSCF-PT2 Calculations with Cold Ion Spectroscopy

T. K. Roy, V. Kopysov, A. Pereverzev, J. Šebek,R. B. Gerber,* and O. V. Boyarkin*
Phys. Chem. Chem. Phys. 20, 24894-24901 (2018). ISSN: 1463-9076, https://doi.org/10.1039/C8CP03989E

26. Phosphine-Free Bis(Pyrrolyl)pyridine based NNN-pincer Palladium(II) Complexes as Efficient Catalysts for Suzuki-Miyaura Cross-Coupling Reactions of Aryl Bromides in Aqueous Medium

S. Yadav,A. Singh,N. Rashid,M. Ghotia,**T. K. Roy**,P. P. Ingole,S. Ray,M. M. Shaikhand C. Dash
ChemistrySelect. (2018), 3, 9469-9475, ISSN**:** 2365-6549, https://doi.org/10.1002/slct.201801647

25. Hypochlorite-Mediated Modulation of Photoinduced Electron Transfer in a Phenothiazine-Boron dipyrromethene Electron Donor-Acceptor Dyad: A Highly Water Soluble "Turn-On" Fluorescent Probe for Hypochlorite

D. Soni, N. Duvva, D. Badgurjar, **T. K. Roy,** S. Nimesh, G. Arya. L. Giribabu, R. Chitta
Chem. Asian. J., 13, 1594-1608, (2018), ISSN**:** 1861-4728, https://doi.org/10.1002/asia.201800349

24. Synthesis of Spirooxindoles through Cyclocondensation of Isatin and Cyclic 1,3-Diones

    R. Joshi, A. Kumawat, S. Singh, **T. K. Roy**, R. T. Pardasani,
    J. Heterocycl. Chem., 55, 1783-1790 (2018), ISSN: 1943-5193, https://doi.org/10.1002/jhet.3217

23. Catalyst-Controlled Structural Divergence: Selective Intramolecular 7-*endo-dig* and 6-*exo-dig* Post-Ugi Cyclization for the Synthesis of Benzoxazepinones and Benzoxazinones

    K. Singh, B. K. Malviya**, T. K. Roy**, V. S. Mithu, V. K. Bhardwaj, V. P. Verma, S. S. Chimni, S. Sharma
    J. Org. Chem, 83, 1, 57-68, (2018), ISSN: 0022-3263.https://doi.org/10.1021/acs.joc.7b02123

22. Azo-dyes based small bifunctional molecules for metal chelation and controlling amyloid formation

    M. Rana, H. J. Cho, **T. K. Roy** , L. M. Mirica, A. K. Sharma*,
    Inorganica Chim. Acta, 471, 419-429, (2017), ISSN: 0020-1693, https://doi.org/10.1016/j.ica.2017.11.029

21. Synthesis of Diverse Nitrogen Heterocycles via Palladium-Catalyzed Tandem Azide–Isocyanide Cross-Coupling/Cyclization: Mechanistic Insight using Experimental and Theoretical Studies

    A. J. Ansari, R. S. Pathare, A. K. Maurya, V. K. Agnihotri, S. Khan, **T. K Roy,*** D. M. Sawant,* and R. T. Pardasani*
    Adv. Synth. Catal., 360, 2, 290-297, (2017), ISSN: 1615-4150, https://doi.org/10.1002/adsc.201700928

20. A Decapeptide Hydrated by Two Waters: Conformers Determined by Theory and Validated by Cold Ion Spectroscopy

    T. K. Roy, N. S. Nagornova, O. V. Boyarkin and R. B. Gerber
    J. Phys. Chem. A.121, 48, 9401-9408, (2017) ISSN: 1520-5215, https://doi.org/10.1021/acs.jpca.7b10357

19. Hypochlorite promoted inhibition of photo-induced electron transfer in phenothiazine-borondipyrromethene donor-acceptor dyad: A cost-effective and metal-free “turn-on” fluorescent chemosensor for hypochlorite

    D. Soni, S. Gangada, N. Duvva, **T. K. Roy**, S. Nimesh, G. Arya, G. Lingamallu and R. Chitta
    New J. Chem., 41, 5322-5333, (2017), ISSN: 1144-0546, https://doi.org/10.1039/C7NJ00516D

18. A catalyst-free one-pot multicomponent synthesis of spirobenzimidazoquinazolinones via Knoevenagel-Michael-Imine pathway: A microwave assisted approach

    P. Maloo, **T. K. Roy**, D. Sawant, R. T. Pardasani and M. M. Salunkhe.
    RSC Advances, 6, 41897 (2016). ISSN: 1523-7060, https://doi.org/10.1039/C6RA05322J

17. Ruthenium catalyzed intramolecular C-S coupling reactions: Synthetic scope and mechanistic insights

    S. Sharma, R. S. Pathare, A. K. Maurya, K. Gopal, **T. K. Roy**, D. M. Sawantand R. T. Pardasani
    Organic Letters, 18, 365, (2016), ISSN: 1523-7060, https://doi.org/10.1021/acs.orglett.5b03185

16. First-Principles Anharmonic Quantum Calculations for Peptides Spectroscopy: VSCF Calculations and Comparison with Experiment

    T. K. Roy, R. Sharma and R. B. Gerber
    Phys. Chem. Chem. Phys. 18, 1607 (2016). ISSN: 1463-9076, https://doi.org/10.1039/C5CP05979H

15. Mechanistic Studies of Malonic Acid-Mediated in situ Acylation

    K. Chandra, J. N. Naoum, **T. K. Roy**, C. Gilon, R. B. Gerber and A. Friedler
    Biopolymers, 104, 495 (2015). ISSN: 1097- 0282, https://doi.org/10.1002/bip.22654

14. Conformational Structures of a Decapeptide Validated by First-Principles Calculations and Cold Ion Spectroscopy

    T. K. Roy, V. Kopysov, N. S. Nagornova, T. R. Rizzo, O. V. Boyarkin and R. B. Gerber
    ChemPhysChem, 16, 1374 (2015). ISSN: 1439- 7641, https://doi.org/10.1002/cphc.201500085

13. Approximate First Principles Anharmonic Calculations of Polyatomic Spectra using MP2 and B3LYP Potentials: Comparisons with Experiment

    T. K. Roy, T. C. Jr. and R. B. Gerber
    J. Phys. Chem. A, 118, 6730, (2014). ISSN: 1520-5215, https://doi.org/10.1021/jp5060155

12. A Tandem In Situ Peptide Cyclization through Trifluoroacetic Acid Cleavage

    K. Chandra, **T. K. Roy**, D. E. Shalev, A. Loyter,C. Gilon R. B. Garber, A. Friedler
    Angew. Chem. Int. Ed., 53, 9450, (2014). ISSN: 1521- 3773, https://doi.org/10.1002/ange.201402789

11. A Highly Efficient *in situ* Acetylation Approach for Diverse Polyfunctionalized Complex Network

    K. Chandra, **T. K. Roy**, J. Naoum, C. Gilon, R. B. Garber and A. Friedler
    Org. Biomol. Chem. 12, 1879 (2014). ISSN: 1477-0520, https://doi.org/10.1039/C3OB42096E

10. Vibrational self-consistent field calculations of spectroscopy of biological molecules

    T. K. Roy and R. B. Gerber.
    Phys. Chem. Chem. Phys.15, 468 (2013). ISSN: 1463-9076, https://doi.org/10.1039/C3CP50739D

9. A comparative study of independent particle model based approaches for thermal averages

    S. Banik, **T. K. Roy** and M. D. Prasad,
    J. Chem. Sci. 125, 1267 (2013). ISSN: 0974-3626, https://doi.org/10.1007/s12039-013-0484-9

8. MOF-FF – A flexible first principles derived Force Field for Metal-Organic Frameworks

    S. Bureekaew, S. Amirjalayer, M. Tafipolsky, C. Spickermann, **T. K. Roy**and R. Schmid
    Physica Status Solidi (b) 250, 1128 (2013). ISSN: 1521- 3951, https://doi.org/10.1002/pssb.201248460

7. Development of a new variational principle for thermal density matrices

    T. K. Royand M. D. Prasad.
    J. Chem. Phys. 134, 214110 (2011). ISSN: 1089-7690, https://doi.org/10.1063/1.3592777

6. Functionalization of the terminal carbon atoms of the hydroxyl terminated polybutadiene by polyazido nitrogen rich molecules

    R. M. Shankar, **T. K. Roy**and T. Jana
    Bull. Mater. Sci., 34, 745 (2011). ISSN: 0250-4707, https://doi.org/10.1007/S12034-011-0190-5

5. Terminal Functionalized Hydroxyl-Terminated: An energytic Binder for propellant

   R. M. Shankar, **T. K. Roy**and T. Jana.
   J. Appl. Poly. Sci. 114, 732 (2009). ISSN: 1097-4628, https://doi.org/10.1002/APP.30665

4. On some strategies to design new high energy density molecules

   T. Mondal, B. Saritha, S. Ghanta, **T. K. Roy**, S. Mahapatra and M. D. Prasad
   Theochem, 897, 42 (2009). ISSN: 0166-1280, https://doi.org/10.1016/j.theochem.2008.11.013

3. Effective harmonic oscillator description of anharmonic molecular vibrations

   T. K. Roy and M. D. Prasad
   J. Chem. Sci. 121, 805 (2009). ISSN: 0974-3626, https://doi.org/10.1007/s12039-009-0095-7

2. A thermal self-consistent field theory for the calculation of molecular vibrational partition functions

   T. K. Royand M D. Prasad.
   J. Chem. Phys. 131, 114102 (2009). ISSN: 0021-9606, https://doi.org/10.1063/1.3213568

- Conformational preferences of mono-substituted cyclohydronitrogens: A theoretical Study

  T. K. Roy, S. Ghanta, T. Mondal, B. Saritha, S. Mahapatra and M. D. Prasad.
  Theo. chem, 822, 145 (2007). ISSN: 0166-1280, https://doi.org/10.1016/j.theochem.2007.08.003

b. **Books**

c. **Chapter in books**

1 (International)

Development of Computational Tools for Diverse Applications of Metal Organic Frameworks: Challenges and Outlooks", Bukhvalov Danil, Pawan Kumar, Abhinav Gondhi, Tapta Kanchan, Roy and Ki-Hyun Kim, Central West Publishing, Australia, ISSN: 978-1-925823-57-8 (2019)

d. **Articles/Research Paper in Books**

e. **Conference Proceedings**

Conference / Workshops/Training Organized:

- 1 international conference, 1 national conference, 2 lecture series, 3 national science day

Creation of ICT Mediated Teaching Learning Pedagogy and Content:

Conference/Workshops/Training attended as Faculty Member:

8

Invited Lectures/Resource Persons (Selected)

- Invited Speaker: First International Conference on Impending Inquisitions in Humanities and Sciences, KLH Hyderabad, 28-30 November, 2022
- Invited Speaker: ERTCS 2020, 24-26 July, 2020
- Resource Person: Faculty Development Program, Department of Chemistry, Jammu University Year: 2018, 2021, 2023
- Invited Speaker: Theoretical Chemistry Symposium, TCS-2019, International Conference, 13th to 16th February, 2019
- Oral Presentation: VI Rajasthan Science Congress, October 13-15, 2018 at Central University of Rajasthan.
- Invited Speaker: International Conference on Frontiers at the Chemistry-Applied Sciences Interface", Organized by University of Rajasthan, July-23-24, 2017, Title: Going solvated: Intrinsic Structures of a Micro-solvated Decapeptide Determined by Theory and Cold-ion Spectroscopy
- Invited Speaker: Theoretical Chemistry Symposium, TCS-2016, International Conference, 14th to 17th December, 2017, University of Hyderabad, IICT & IIIT, Hyderabad, Title: Conformationally Resolved Structures of Large Biological Molecules Validated by First Principles Based Anharmonic Calculations
- International Conference on Frontiers at the Chemistry-Applied Sciences Interface, April-25-26, 2016, University of Rajasthan, Title: Conformational Structures of a Decapeptide Validated by First-Principles Calculations and Cold Ion Spectroscopy
- J & K Science Congress, March 2-4, 2017 at University of Jammu, Title: Conformationally resolved 3d-structures and spectroscopy of large bio-molecules using quantum mechanical anharmonic calculations
- Advances in Chemical Sciences and Thermodynamics, December 2-3, 2016, University of Jammu, Title: Variational approach of thermodynamic quantities.

Resource Person: Orientation Program, Department of Chemistry, University of Jammu (December, 2018)

Research Projects (Major Grants/Research Collaboration):

- DST-MATRICS grant, 2022-2025 (6.6 lacs) : Ongoing
- DST-EMR grant, 2018-2021 (55.1 lacs) : Completed
- UGC-startup grant, 2017-2020 (10 lacs) : Completed
- University startup grant from CU Jammu (2 lacs) : Completed

Awards and Distinctions:

- CSIR Junior Research Fellowship (JRF) – by qualifying the All India National Eligibility Test (NET) conducted by CSIR-UGC, INDIA, in 2005.
- Post-doctoral fellowship by SFB 558, Ruhr University, Germany.
- Received prestigious PBC fellowship for post doctoral research by Government of Israel.

Association with Professional Bodies:

- CRSI Life Member

Other Activities: